Influence of the biquadratic interaction to magnetic surface reconstruction

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The surface spin ordering is studied in a ferromagnetic crystal where spins interact both by bilinear and biquadratic interaction. The surface spin configuration is unstable with respect to ferromagnetic alignment for certain values of parameters leading to so-called surface magnetic reconstruction. It is shown that biquadratic interaction enhances the reconstruction. The energy of surface excitations is calculated and it is shown to be much lower than the energy of bulk excitations in presence of surface reconstruction, while the surface Goldstone mode appears only in the case of vanishing external field and anisotropy. Mean field calculation is presented for the study of the behavior of surface magnetization. [S0163-1829(99)00126-5]

I. INTRODUCTION

During the last several years, interest has grown for the study of magnetic surfaces, thin films, and multilayered structures, both from experimental and theoretical points of view.[1] There exist nowadays modern experimental techniques [low-energy electron diffraction (LEED), nuclear magnetic resonance (NMR)] which enable the precise measurements of the quantities of the local character such as the magnetization or susceptibility. This whole interest, of course, is motivated primarily by the possible application of given materials for memory devices.

One interesting effect related to surfaces is the phenomenon of *magnetic surface reconstruction*. The effect involved means that under certain conditions the spin configuration at the surface could become unstable with respect to the ferromagnetic ordering and transit to a new state with spins tilted with respect to magnetization axis. For the case of the semi-infinite Heisenberg ferromagnet, this phenomenon was studied in detail[2–4] and these studies will be our starting point.

On the other hand, higher-order couplings (for spin $S \geqslant 1$) have been the subject of interest for a long time,[5,6] while the practical interest in biquadratic (more generally, quadrupolar) interaction started about 20 years ago, when this interaction was added to the bilinear Heisenberg one to explain the magnetic properties of the materials like MnAs, UO_2, UP, TbSb, MnO, $\alpha-$MnS, EuSe, rare-earth vanadates, arsenates, and phosphates.[7,8] Moreover, it was shown that there exist materials in which the quadrupolar interaction is the dominant one, like molecular crystals[9] or Jahn-Teller ferroelectric systems.[10] This situation immediately caused a more thorough theoretical study of the system. The most extensive study within the mean-field approximation was performed by Chen and Levy,[11] and studies by more sophisticated techniques (Green's functions, mostly) followed.[12–22] However, all these results dealt only with the bulk materials and this inspired us to perform a study where we shall examine the possibility of surface reconstruction for the case of semi-infinite face-centered-cubic lattice ferromagnet, depending on the external magnetic field, bilinear, and biquadratic Heisenberg interaction.

We shall study the above-described ferromagnet with translational symmetry in XZ plane and Y axis perpendicular to crystal surface. The magnetic moments interact by both bilinear Heisenberg exchange ($I_{\mathbf{nm}}$) and biquadratic exchange ($aI_{\mathbf{nm}}$), where a is the constant of the biquadratic interaction. We shall simplify the model by treating only the interaction between nearest neighbors.

First of all, let us be precise about the notation. The cell's site is defined in terms of layer (plane) index n (starting from zero and increasing along the Y axis) and two-dimensional (2D) vector $\boldsymbol{\rho}$ denoting the position within the plane: $\mathbf{n}=(\boldsymbol{\rho},n)$, and accordingly, for the spin operators $\mathbf{S_n}=\mathbf{S}_{\boldsymbol{\rho}}(n)$. The nearest neighbors approximation will be realized by the assumption

$$I_{\mathbf{n}-\mathbf{m}}=\begin{cases}-I_S & \text{for } n=m=0\\ I & \text{otherwise}\end{cases}.$$

This leads to the Hamiltonian of the system in the form ($\boldsymbol{\lambda}_n$ counts the nearest neighbors in the nth layer)

$$H=\frac{I_S}{2}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_0}\mathbf{S}_{\boldsymbol{\rho}}(0)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(0)+\frac{aI_S}{2}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(\mathbf{S}_{\boldsymbol{\rho}}(0)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(0))^2-I\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_1}\mathbf{S}_{\boldsymbol{\rho}}(0)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(1)-aI\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(\mathbf{S}_{\boldsymbol{\rho}}(0)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(1))^2$$
$$-\frac{I}{2}\sum_{n,m\geqslant 1}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_m}\mathbf{S}_{\boldsymbol{\rho}}(n)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(m)-\frac{aI}{2}\sum_{n,m\geqslant 1}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(\mathbf{S}_{\boldsymbol{\rho}}(n)\mathbf{S}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(m))^2+H_{AB}+H_{AS}-g\mu_B\mathcal{H}\sum_n\sum_{\boldsymbol{\rho}}\hat{S}^z_{\boldsymbol{\rho}}(n). \quad (1)$$

The meaning of all of the sums is clear, while H_{AB} and H_{AS} include the bulk and surface single-ion anisotropy. The bulk anisotropy term we take in the form

$$\hat{H}_{AB}=-D\sum_{n\geqslant 1}\sum_{\boldsymbol{\rho}}(\hat{S}^{z}_{\boldsymbol{\rho}}(n))^{2} \tag{2}$$

{Although in the bulk systems with cubic symmetry the allowed single-ion anisotropy is of the form $-D[(S_x)^4+(S_y)^4+(S_z)^4]$, one can demonstrate that its contribution is proportional to $(\hat{S}^z)^2$ in the approximation quadratic in Bose operators.} Following Ref. 4 we introduce the surface anisotropy as

$$\hat{H}_{AS}=-\sum_{\boldsymbol{\rho},n=0}[K_x(\hat{S}^{x}_{\boldsymbol{\rho}}(0))^2+K_y(\hat{S}^{y}_{\boldsymbol{\rho}}(0))^2+K_z(\hat{S}^{z}_{\boldsymbol{\rho}}(0))^2]$$

which can be cast into the form

$$\hat{H}_{AS}=-D_S\sum_{\boldsymbol{\rho},n=0}(\hat{S}^{z}_{\boldsymbol{\rho}}(0))^2 -\frac{\Delta K}{2}\sum_{\boldsymbol{\rho},n=0}[(\hat{S}^{x}_{\boldsymbol{\rho}}(0))^2-(\hat{S}^{y}_{\boldsymbol{\rho}}(0))^2], \tag{3}$$

where $D_S=K_z-(K_x+K_y)/2$; $\Delta K=K_x-K_y$.

Let us finally comment on the values of the parameters. The biquadratic interaction is important for $S\geqslant 1$, so we shall concentrate on these values, with particular attention paid to the case $S=1$, when most of the expressions are simplified. However, the bulk studies indicate that for $a>1$, more complex configurations arise, so we shall limit our calculations to the range $0\leqslant a\leqslant 1$.

The structure of the paper is as follows: The Hamiltonian of the system in the presence of surface reconstruction is analyzed in Sec. II, where the local frame for surface spins is introduced. The Hamiltonian is stabilized leading to the conditions for the reconstruction. Boson representation which is used for the study of elementary excitations is introduced in Sec. III. The results are summarized in Sec. IV where also a mean-field study is outlined.

II. THE HAMILTONIAN OF THE SYSTEM IN THE PRESENCE OF SURFACE RECONSTRUCTION

We shall assume that the ground state in the bulk is defined by the ordering of spins along the Z axis, while the possible surface reconstruction manifests itself by the deviation of surface spins from the Z direction for the angle θ within the XZ plane. The surface is divided into two sublattices denoted a and b, and although we shall formally work with sublattices, we remember that the only difference occurs in the surface layer where a spins deviate for the angle θ while b spins deviate for the angle $-\theta$. The spin configuration in the surface layer is presented in Fig. 1. Let us now define the local frame, where the spins are denoted by primed quantities:

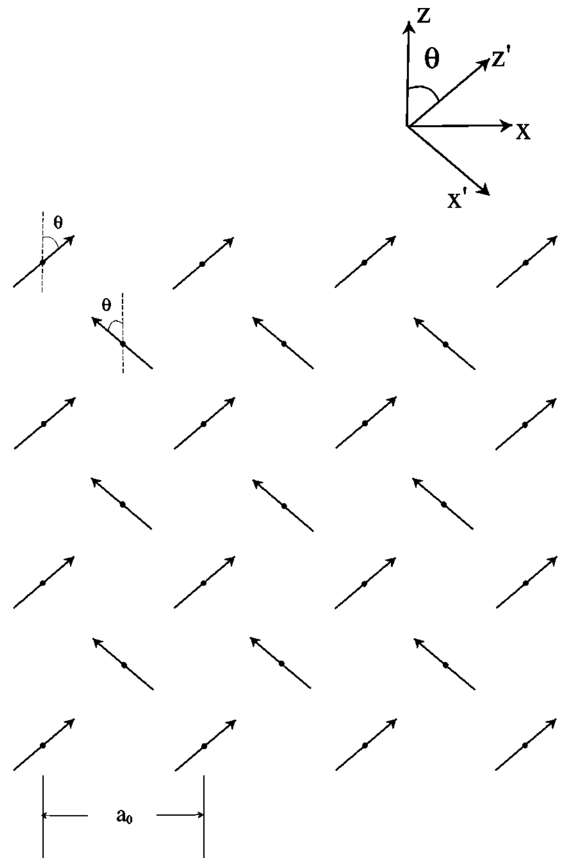

FIG. 1. Spin configuration of the surface layer in the presence of magnetic surface reconstruction. The axes of the local frame are denoted.

$$\hat{S}^{x}_{\boldsymbol{\rho}_{a/b}}(0)=\cos\theta\hat{S}^{x'}_{\boldsymbol{\rho}_{a/b}}(0)\pm\sin\theta\hat{S}^{z'}_{\boldsymbol{\rho}_{a/b}}(0),$$

$$\hat{S}^{y}_{\boldsymbol{\rho}_{a/b}}(0)=\hat{S}^{y'}_{\boldsymbol{\rho}_{a/b}}(0),$$

$$\hat{S}^{z}_{\boldsymbol{\rho}_{a/b}}(0)=\mp\sin\theta\hat{S}^{x'}_{\boldsymbol{\rho}_{a/b}}(0)+\cos\theta\hat{S}^{z'}_{\boldsymbol{\rho}_{a/b}}(0), \tag{4}$$

$$\text{for}\quad n\geqslant 1\qquad \hat{S}_{\boldsymbol{\rho}}(n)=\mathbf{S}'_{\boldsymbol{\rho}}(n). \tag{5}$$

We shall present here the calculation details for the bilinear interaction only, due to the cumbersome form of the expressions for the biquadratic interaction.

The quantization axis is Z' and it is given by the relation $\hat{S}^{z'}_{\boldsymbol{\rho}}(n)|0\rangle'_{\boldsymbol{\rho}_n}=S|0\rangle'_{\boldsymbol{\rho}_n}$ for $n=0,1,2,\ldots$. It is clear that this last relation makes no distinction between a and b sites.

From the relations (4) and (5) one concludes that the reconstruction affects only the terms of the Hamiltonian which describe the interaction of spins at the surface $[\hat{H}(0,0)]$ and between the surface and first bulk layer $[\hat{H}(0,1)]$:

$$\hat{H}(0,0)+\hat{H}(0,1)=\frac{I_S}{2}\sum_{\boldsymbol{\rho}_a,\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}\{\cos 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}(0)+\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}(0)]+\hat{S}^{y'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}(0)+\sin 2\theta[\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}(0)$$
$$-\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_b}(0)]\}+\frac{I_S}{2}\sum_{\boldsymbol{\rho}_b,\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}\{\cos 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}(0)+\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}(0)]+\hat{S}^{y'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}(0)$$
$$+\sin 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}(0)-\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_a}(0)]\}-I\sum_{\boldsymbol{\rho}_a,\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}\{[\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)+\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)]\cos\theta$$
$$+\hat{S}^{y'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)+\sin\theta[\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)-\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)]\}-I\sum_{\boldsymbol{\rho}_b,\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}\{[\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)$$
$$+\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)]\cos\theta+\hat{S}^{y'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)]-\sin\theta[\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)-\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)]\} \tag{6}$$

Possible values of the reconstruction angle θ are determined from the stabilization of the Hamiltonian (6). We shall minimize over θ the energy of the new ground state $|0\rangle' =\Pi_{\boldsymbol{\rho}_0}\Pi_{\boldsymbol{\rho}'_1}|0\rangle'_{\boldsymbol{\rho}_0}|0\rangle'_{\boldsymbol{\rho}'_1}$. It can be easily demonstrated that the ground-state energy per site equals

$$E_o(\theta)=2S^2I_S\cos 2\theta-4S^2I\cos\theta-g\mu_B\mathcal{H}S\cos\theta. \tag{7}$$

Introducing $J_S=4I_SS$; $J=4SI$; $h=g\mu_B\mathcal{H}$, we obtain the basic condition

$$\sin\theta(2J_s\cos\theta-J-h)=0. \tag{8}$$

This equation possesses two solutions. The first one,

$$\theta=0,$$

corresponds to the situation when no reconstruction occurs. The solution which allows the possibility of the reconstruction is

$$\cos\theta=\frac{J+h}{2J_S}. \tag{9}$$

It follows from Eq. (9) that the reconstruction is possible if $J_S>J_S^c$, where the critical value of the exchange is given by

$$J_S^c=\frac{J+h}{2}. \tag{10}$$

Let us mention that the relation (8) can be obtained also by the bosonization of ''primed'' spin operators (within Bloch approximation) and elimination of terms linear in Bose operators, arising from the combination $\sim\hat{S}^{x'}_{\boldsymbol{\rho}}(0)\hat{S}^{z'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(i)$, $i=0,1$, in the Hamiltonian (6). After this elimination, we are left with the Hamiltonian which contributes to the quadratic terms in Bose operators in the form

$$\hat{H}_2(0,0)+\hat{H}_2(0,1)=\frac{I_S}{2}\sum_{\boldsymbol{\rho}_a,\boldsymbol{\rho}_a+\boldsymbol{\lambda}_0}\{\cos 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_0}(0)+\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_0}(0)]+\hat{S}^{y'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_0}(0)\}$$
$$+\frac{I_S}{2}\sum_{\boldsymbol{\rho}_b,\boldsymbol{\rho}_b+\boldsymbol{\lambda}_0}\{\cos 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_0}(0)+\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_0}(0)]+\hat{S}^{y'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_0}(0)\}$$
$$-I\sum_{\boldsymbol{\rho}_a,\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}\{\cos\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)+\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)]+\hat{S}^{y'}_{\boldsymbol{\rho}_a}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_a+\boldsymbol{\lambda}_1}(1)\}$$
$$-I\sum_{\boldsymbol{\rho}_b,\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}\{\cos\theta[\hat{S}^{x'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{x'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)+\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{z'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)]+\hat{S}^{y'}_{\boldsymbol{\rho}_b}(0)\hat{S}^{y'}_{\boldsymbol{\rho}_b+\boldsymbol{\lambda}_1}(1)\}$$
$$-h\cos\theta\left(\sum_{\boldsymbol{\rho}_a}\hat{S}^{z'}_{\boldsymbol{\rho}_a}(0)+\sum_{\boldsymbol{\rho}_b}\hat{S}^{z'}_{\boldsymbol{\rho}_b}(0)\right). \tag{11}$$

In the above Hamiltonian, the summations over $\boldsymbol{\rho}_a$ and $\boldsymbol{\rho}_b$ in the surface layer can be written as a unique sum over $\boldsymbol{\rho}$, according to the definition of primed quantities. We see that, within the framework of the given approximation, surface reconstruction leads to the anisotropic interaction at the surface and between the surface layer and first layer, while it does not change two-dimensional (2D) lattice, neither will it influence 2D Brillouin zone (BZ).

Regrouping all the terms with bilinear interaction we obtain the spin Hamiltonian which contributes to second-order Hamiltonian in Bose operators:

$$\hat{H}_2=\frac{I_S}{2}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_0}\{\cos 2\theta[\hat{S}^{x'}_{\boldsymbol{\rho}}(0)\hat{S}^{x'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(0)+\hat{S}^{z'}_{\boldsymbol{\rho}}(0)\hat{S}^{z'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(0)]+\hat{S}^{y'}_{\boldsymbol{\rho}}(0)\hat{S}^{y'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_0}(0)\}-h\cos\theta\sum_{\boldsymbol{\rho}}\hat{S}^{z'}_{\boldsymbol{\rho}}(0)$$
$$-I\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_1}\{\cos\theta[\hat{S}^{x'}_{\boldsymbol{\rho}}(0)\hat{S}^{x'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(1)+\hat{S}^{z'}_{\boldsymbol{\rho}}(0)\hat{S}^{z'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(1)]+\hat{S}^{y'}_{\boldsymbol{\rho}}(0)\hat{S}^{y'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_1}(1)\}$$
$$-\frac{I}{2}\sum_{m,n\geqslant 1}\sum_{\boldsymbol{\rho},\boldsymbol{\rho}+\boldsymbol{\lambda}_m}[\hat{S}^{x'}_{\boldsymbol{\rho}}(n)\hat{S}^{x'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(m)+\hat{S}^{z'}_{\boldsymbol{\rho}}(n)\hat{S}^{z'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(m)+\hat{S}^{y'}_{\boldsymbol{\rho}}(n)\hat{S}^{y'}_{\boldsymbol{\rho}+\boldsymbol{\lambda}_m}(m)]-h\sum_{\boldsymbol{\rho},n\geqslant 1}\hat{S}^{z'}_{\boldsymbol{\rho}}(n) \tag{12}$$

This concludes the part concerning the contribution of the bilinear interaction.

A similar procedure can be applied to biquadratic and anisotropic parts of the Hamiltonian, where again, only the terms contributing to the Hamiltonian quadratic in Bose operators are retained. We are not going to write them explicitly, but only quote the results.

The ground-state energy including the contributions of the complete Hamiltonian (1) has the following form:

$$E_o(\theta)=\frac{1}{2}aJ_S(2S-1)^2\cos^4\theta+\frac{1}{2}[2J_S(1-a/2)$$
$$-aJ_S(2S-1)^2-aJ/2(2S-1)^2+(2S-1)$$
$$\times(\Delta K/2-D_S)]\cos^2\theta-[J(1-a/2)+h]\cos\theta. \tag{13}$$

Deriving this expression over θ, we obtain the condition for the extreme values of energy $\partial E_o(\theta)/\partial\theta=0$, with one solution corresponding to unreconstructed surface:

$$\sin\theta=0, \tag{14}$$

while the reconstruction angle θ is defined by a cubic equation in terms of $\cos\theta$:

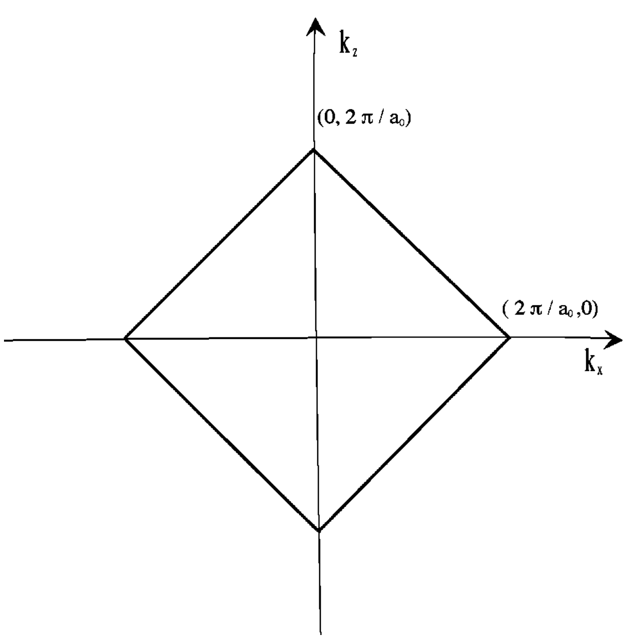

FIG. 2. Two-dimensional I Brillouin zone.

$$2aJ_S(2S-1)^2\cos^3\theta+[2J_S(1-a/2)-aJ_S(2S-1)^2$$
$$-aJ/2(2S-1)^2+(2S-1)(\Delta K/2-D_S)]$$
$$\times\cos\theta-[J(1-a/2)+h]=0. \tag{15}$$

The discussion of the solutions of this equation will be given in the next section.

The transition to Bose operators is realized in such a way to include only the terms contributing to second-order Hamiltonian. For that purpose, we use the following representation:

$$\hat{S}^{x'}_{\boldsymbol{\rho}}(n)=\sqrt{\frac{S}{2}}[\hat{a}^+_{\boldsymbol{\rho}}(n)+\hat{a}_{\boldsymbol{\rho}}(n)],$$

$$\hat{S}^{y'}_{\boldsymbol{\rho}}(n)=i\sqrt{\frac{S}{2}}[\hat{a}^+_{\boldsymbol{\rho}}(n)-\hat{a}_{\boldsymbol{\rho}}(n)],$$

$$\hat{S}^{z'}_{\boldsymbol{\rho}}(n)=S-\hat{a}^+_{\boldsymbol{\rho}}(n)\hat{a}_{\boldsymbol{\rho}}(n). \tag{16}$$

This choice of boson representation is valid as long as $\theta\neq\pi/2$, i.e., in the cases with no complete antiferromagnetic ordering. In the case of antiferromagnetic ordering, the introduction of two types of boson operators corresponding to different ground states would be necessary. The quadratic terms must be written in the following way:

$$(\hat{S}^{z'}_{\mathbf{n}})^2=S^2-(2S-1)\hat{a}^+_{\mathbf{n}}\hat{a}_{\mathbf{n}},$$

$$(\hat{S}^{-'}_{\mathbf{n}})^2=(2S-1)(\hat{a}^+_{\mathbf{n}})^2,$$

$$(\hat{S}^{+'}_{\mathbf{n}})^2=(2S-1)(\hat{a}_{\mathbf{n}})^2. \tag{17}$$

This representation is obtained by taking into account the contribution of the normal order of higher terms to second-order terms, and, what is more important, it leads to the same results as the equations linearized in spins. (Please notice that the bosonization is performed in the local frame.) After the transition to Bose operators (16) and (17), we can introduce two-dimensional Fourier transforms:

$$\hat{a}_{\boldsymbol{\rho}}(l)=\frac{1}{\sqrt{N_xN_z}}\sum_{\mathbf{k}_\parallel}a_{\mathbf{k}_\parallel}(l)e^{i\mathbf{k}_\parallel\boldsymbol{\rho}}, \tag{18}$$

where

$$\boldsymbol{\rho}=n_x\frac{a_0}{2}\mathbf{e}_x+n_z\frac{a_0}{2}\mathbf{e}_z$$

is the same for both $\theta=0$ and $\theta\neq 0$.

The summation over $\mathbf{k}_\parallel$ goes over 2D BZ, i.e.,

$$-\frac{2\pi}{a_o}\leqslant k_x\leqslant \frac{2\pi}{a_o},\quad -\frac{2\pi}{a_o}\leqslant k_z\leqslant \frac{2\pi}{a_o},$$

whose shape is presented in Fig. 2.

In this way we obtain the total Hamiltonian of the system, quadratic in bose operators:

$$\begin{aligned}\hat{H}_{tot}=&\sum_{\mathbf{k}_\parallel}\omega_S(\mathbf{k}_\parallel)a^+_{\mathbf{k}_\parallel}(0)a_{\mathbf{k}_\parallel}(0)+\frac{1}{2}\sum_{\mathbf{k}_\parallel}\alpha_S(\mathbf{k}_\parallel)[a^+_{\mathbf{k}_\parallel}(0)a^+_{-\mathbf{k}_\parallel}(0)+\text{H.c.}]+\sum_{\mathbf{k}_\parallel}\omega_{S1}\gamma^+(\mathbf{k}_\parallel)[a^+_{\mathbf{k}_\parallel}(0)a_{\mathbf{k}_\parallel}(1)+\text{H.c.}]\\&+\sum_{\mathbf{k}_\parallel}\alpha_{S1}\gamma^+(\mathbf{k}_\parallel)[a^+_{\mathbf{k}_\parallel}(0)a^+_{-\mathbf{k}_\parallel}(1)+\text{H.c.}]+\sum_{\mathbf{k}_\parallel}\omega_1(\mathbf{k}_\parallel)a^+_{\mathbf{k}_\parallel}(1)a_{\mathbf{k}_\parallel}(1)-\frac{1}{2}\sum_{\mathbf{k}_\parallel}\alpha_1[a^+_{\mathbf{k}_\parallel}(1)a^+_{-\mathbf{k}_\parallel}(1)+\text{H.c.}]\\&+\sum_{l\geqslant 2}\sum_{\mathbf{k}_\parallel}\omega(\mathbf{k}_\parallel)a^+_{\mathbf{k}_\parallel}(l)a_{\mathbf{k}_\parallel}(l)-\tilde{J}\sum_{l\geqslant 2}\sum_{\mathbf{k}_\parallel}\gamma^+(\mathbf{k}_\parallel)[a^+_{\mathbf{k}_\parallel}(l)a_{\mathbf{k}_\parallel}(l-1)+\text{H.c.}].\end{aligned}\tag{19}$$

The following notation has been introduced here:

$$\begin{aligned}\omega_S(\mathbf{k}_\parallel)=&(h+J)\cos\theta-J_S\cos 2\theta+J_Sa\left[-3(2S-1)^2(\cos\theta)^4+3(2S-1)^2(\cos\theta)^2+(\cos\theta)^2-\frac{1}{2}(2S-1)^2-\frac{1}{2}\right]\\&-aJ\left[-\frac{3}{4}(2S-1)^2(\cos\theta)^2+\frac{1}{2}\cos\theta+\frac{1}{4}(2S-1)^2\right]+\gamma(\mathbf{k}_\parallel)\{J_S(\cos\theta)^2+2J_Sa[(2S-1)^2\cos 4\theta-(3S^2-3S+1)\\&\times(\cos\theta)^2J]\}+\frac{2S-1}{2}\left\{D_S[3(\cos\theta)^2-1]+\frac{3}{4}\Delta K(\sin\theta)^2\right\},\end{aligned}$$

$$\begin{aligned}\alpha_S(\mathbf{k}_\parallel)=&-J_S(\sin\theta)^2\left\{\gamma(\mathbf{k}_\parallel)\left[1+a\left(2(2S-1)^2(\cos\theta)^2-\frac{1}{2}(2S-1)^2-\frac{1}{2}\right)\right]-(2S-1)^2a\left((\cos\theta)^2-\frac{J}{4J_S}\right)\right\}\\&-\frac{2S-1}{2}\left(D_S(\sin\theta/2)^2+\frac{\Delta K}{2}[(\cos\theta/2)^2+1]\right),\end{aligned}$$

$$\omega_{S1}=-J(\cos\theta/2)^2\left(1+\frac{a}{2(\cos\theta/2)^2}[(2S-1)^2(\cos\theta)^2+2S(S-1)\cos\theta-2S^2+2S-1]\right),$$

$$\alpha_{S1}=J(\sin\theta/2)^2\left(1-\frac{a}{2(\sin\theta/2)^2}[(2S-1)^2(\cos\theta)^2-(2S^2-2S+1)\cos\theta-2S(S-1)]\right),$$

$$\omega_1(\mathbf{k}_\parallel)=J\cos\theta+2\tilde{J}+h+\frac{aJ}{2}\left(\frac{3}{2}(2S-1)^2(\cos\theta)^2-\cos\theta-\frac{1}{2}(2S-1)^2\right)-\tilde{J}\gamma(\mathbf{k}_\parallel)+(2S-1)D,$$

$$\alpha_1=\frac{aJ}{4}(2S-1)^2(\sin\theta)^2,$$

$$\omega(\mathbf{k}_\parallel)=h+3\tilde{J}-\tilde{J}\gamma(\mathbf{k}_\parallel)+(2S-1)D,$$

$$\tilde{J}=J[1+2aS(S-1)],$$

$$\gamma(\mathbf{k}_\parallel)=\cos\frac{k_za_o}{2}\cos\frac{k_xa_o}{2},$$

$$\gamma^+(\mathbf{k}_\parallel)=\frac{1}{2}\left(\cos\frac{k_za_o}{2}+\cos\frac{k_xa_o}{2}\right).$$

Finally, let us note that in the case of reconstruction $\theta \neq 0$, one can eliminate the external field from the expression for $\omega_S(\mathbf{k}_\parallel)$, leading to

$$\omega_S(\mathbf{k}_\parallel)=\tilde{J}_S[1+\gamma(\mathbf{k}_\parallel)(\cos\theta)^2]-J_S a(2S-1)^2[(\sin\theta)^2 +2\gamma(\mathbf{k}_\parallel)(\cos\theta)^2](\sin\theta)^2-\frac{2S-1}{2}\{D_S(\sin\theta)^2 -\Delta K[(\sin\theta)^2+2]\}-\frac{Ja}{4}(2S-1)^2(\sin\theta)^2, \tag{20}$$

$$\tilde{J}_S=J_S[1+2aS(S-1)].$$

III. SURFACE EXCITATIONS IN THE PRESENCE OF SURFACE RECONSTRUCTION

Starting from the boson Hamiltonian (19), we are going to determine in this section the dispersion law of surface (and bulk) spin waves in a closed form.

Due to ''anomalous'' coupling of the form $\hat{a}\hat{a}$ and $\hat{a}^+\hat{a}^+$, our initial point will be the equations of motion for ''two-component'' operators

$$\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l,t) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l,t) \end{pmatrix},$$

which shall be immediately written in the energy representation, i.e., in terms of the Fourier transforms:

$$\hat{a}_{\mathbf{k}_\parallel}(l,\Omega)=\frac{1}{2\pi}\int \hat{a}_{\mathbf{k}_\parallel}(l,t)e^{i\Omega t}dt.$$

A simple calculation gives:

for $l=0$,

$$\begin{pmatrix} \Omega-\omega_S(\mathbf{k}_\parallel) & -\alpha_S(\mathbf{k}_\parallel) \\ \alpha_S(\mathbf{k}_\parallel) & \Omega+\omega_S(\mathbf{k}_\parallel) \end{pmatrix}\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(0) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(0) \end{pmatrix}+\gamma^+(\mathbf{k}_\parallel) \times\begin{pmatrix} \omega_{S1} & \alpha_{S1} \\ -\alpha_{S1} & -\omega_{S1} \end{pmatrix}\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1) \end{pmatrix}=0 \tag{21}$$

for $l=1$,

$$\begin{pmatrix} \Omega-\omega_1(\mathbf{k}_\parallel) & -\alpha_1 \\ \alpha_1 & \Omega+\omega_1(\mathbf{k}_\parallel) \end{pmatrix}\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1) \end{pmatrix}-\gamma^+(\mathbf{k}_\parallel) \times\begin{pmatrix} \omega_{S1} & \alpha_{S1} \\ -\alpha_{S1} & -\omega_{S1} \end{pmatrix}\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(0) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(0) \end{pmatrix}+\tilde{J}\gamma^+(\mathbf{k}_\parallel)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \times\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(2) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(2) \end{pmatrix}=0, \tag{22}$$

for $l\geqslant 2$,

$$\begin{pmatrix} \Omega-\omega(\mathbf{k}_\parallel) & 0 \\ 0 & \Omega+\omega(\mathbf{k}_\parallel) \end{pmatrix}\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l) \end{pmatrix} +\begin{pmatrix} \tilde{J}\gamma^+(\mathbf{k}_\parallel) & 0 \\ 0 & -\tilde{J}\gamma^+(\mathbf{k}_\parallel) \end{pmatrix}\left[\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l-1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l-1) \end{pmatrix} +\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l+1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l+1) \end{pmatrix}\right]=0. \tag{23}$$

The solutions for $l\geqslant 1$ are written in the form

$$\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l) \end{pmatrix}=\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1) \end{pmatrix}e^{i(l-1)\kappa}, \tag{24}$$

where $\kappa=\alpha+i\eta$ and $\eta\geqslant 0$ in order to keep the amplitude of the surface waves finite. Substituting Eq. (24) into Eq. (23), we obtain two possible values for κ:

$$2\tilde{J}\gamma^+(\mathbf{k}_\parallel)\cos\kappa_1=\omega(\mathbf{k}_\parallel)-\sqrt{\Omega^2},$$

$$2\tilde{J}\gamma^+(\mathbf{k}_\parallel)\cos\kappa_2=\omega(\mathbf{k}_\parallel)+\sqrt{\Omega^2}. \tag{25}$$

For real $\kappa=k_y a_o/2$ (i.e., for $\eta=0$), both solutions lead to the same result for Ω^2, which, in fact, represents the energy of the bulk spin waves:

$$\Omega_B^2=\left(\omega(\mathbf{k}_\parallel)-2\tilde{J}\gamma^+(\mathbf{k}_\parallel)\cos\frac{k_y a_o}{2}\right)^2. \tag{26}$$

This solution is valid for both $\theta\neq 0$ and $\theta=0$ (no reconstruction), the difference appearing in the boundary conditions for the amplitudes of bulk spin waves [Eqs. (21) and (22)], but we are not going to discuss this problem in detail. (The procedure is described in detail in our previous works.[23,24])

The energy of the surface excitations (Ω_S) is defined by two complex solutions $\kappa_{1/2}$, ($\eta_{1/2}>0$). Introducing a new quantity

$$x=-i\cot\frac{\kappa_1+\kappa_2}{2} \tag{27}$$

after simple trigonometric transformations, we obtain Ω_S in terms of x:

$$\Omega_S^2=\frac{(\omega(\mathbf{k}_\parallel))^2}{x^2}+\frac{4\tilde{J}^2(\gamma^+(\mathbf{k}_\parallel))^2}{1-x^2}. \tag{28}$$

The basic problem now is the determination of the quantity x in terms of system parameters and $\mathbf{k}_\parallel$ wave vector from 2D BZ.

It can be easily seen that the general solution of Eq. (23) is of the form

$$\begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(l) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(l) \end{pmatrix} = \begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1) \\ 0 \end{pmatrix} e^{i(l-1)\kappa_1} + \begin{pmatrix} 0 \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1) \end{pmatrix} e^{i(l-1)\kappa_2}$$
$$\equiv \begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1)e^{i(l-1)\kappa_1} \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1)e^{i(l-1)\kappa_2} \end{pmatrix}. \tag{29}$$

After substituting Eq. (29) into Eqs. (22) and (23) and subtracting these two systems of equations, we obtain $[\Delta\omega_1(\mathbf{k}_\parallel)=\omega(\mathbf{k}_\parallel)-\omega_1]$:

$$\begin{pmatrix} \Delta\omega_1(\mathbf{k}_\parallel)-\tilde{J}\gamma^+(\mathbf{k}_\parallel)e^{-i\kappa_1} & \alpha_1 \\ -\alpha_1 & -\Delta\omega_1(\mathbf{k}_\parallel)+\tilde{J}\gamma^+(\mathbf{k}_\parallel)e^{-i\kappa_2} \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(1) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(1) \end{pmatrix} - \gamma^+(\mathbf{k}_\parallel)$$
$$\times \begin{pmatrix} \omega_{S1} & \alpha_{S1} \\ -\alpha_{S1} & -\omega_{S1} \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}_\parallel}(0) \\ \hat{a}^+_{-\mathbf{k}_\parallel}(0) \end{pmatrix} = 0. \tag{30}$$

The relations (30) and (21) give us a system of four homogenous equations for the determination of four amplitudes $\hat{a}_{\mathbf{k}_\parallel}(0), \hat{a}^+_{-\mathbf{k}_\parallel}(0), \hat{a}_{\mathbf{k}_\parallel}(1)$, and $\hat{a}^+_{-\mathbf{k}_\parallel}(1)$. The condition of vanishing of the determinant of the system gives an equation for the determination of x.

The calculation is straightforward, yet cumbersome, so we are not going to present it in detail. Let us only mention that for that purpose we have to use the expression for energy (28) and the following auxilliary relations:

$$e^{-i(\kappa_1+\kappa_2)} = \frac{x-1}{x+1}; \quad e^{-i\kappa_1}+e^{-i\kappa_2} = \frac{\omega(\mathbf{k}_\parallel)}{\tilde{J}\gamma^+(\mathbf{k}_\parallel)} \frac{x-1}{x}$$
$$J\gamma^+(\mathbf{k}_\parallel)(e^{-i\kappa_1}-e^{-i\kappa_2}) = \Omega(x-1). \tag{31}$$

The result is an equation of the sixth order:

$$\Delta(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5 + a_6x^6 = 0, \tag{32}$$

whose coefficients are presented in the Appendix.

The procedure for obtaining the energy of surface excitations is now clear: for a given set of values of system parameters $(J, J_S, D_S, \Delta K, D)$ and a given wave vector $\mathbf{k}_\parallel$, we determine x from Eq. (32) and then the energy $\Omega_S(\mathbf{k}_\parallel)$ from Eq. (28). We must mention that there exists a restriction for x, which can be obtained from Eqs. (25) and (28). Performing an analysis similar to the one explained in detail in the Appendix of Ref. 24, it can be shown that the system allows only the acoustic branches of surface excitations ($\Omega_S \leqslant \Omega_B^{bott}$), for which $\alpha_1 = \alpha_2 = 0$ and

$$x = -\cot\frac{\eta_1+\eta_2}{2}, \quad \text{i.e.,} \quad x < -1. \tag{33}$$

In the next section, we are going to analyze the energies of surface excitations for some values of the system parameters, using Eqs. (28), (32), and (33). One can immediately notice that in our approach to the reconstruction problem, contrary to Ref. 4, there always exists a single branch of surface excitations for given set of parameters. A similar situation occurs for semi-infinite antiferromagnetic, as shown by Wolfram and De Wames[25] for bilinear Heisenberg interaction and in Refs. 23 and 24 for an antiferromagnetic with biquadratic interaction.

Closing this section, let us present the corresponding equations for x and Ω_S for the case with no reconstruction ($\theta=0$). The equation for x becomes a quadratic one:

$$x^2[\omega_S(\mathbf{k}_\parallel)\Delta\omega_S(\mathbf{k}_\parallel) - \tilde{J}^2(\gamma^+(\mathbf{k}_\parallel))^2] + x[J^2(\gamma^+(\mathbf{k}_\parallel))^2$$
$$-(\Delta\omega_S(\mathbf{k}_\parallel))^2] - \omega(\mathbf{k}_\parallel)\Delta\omega_S(\mathbf{k}_\parallel) = 0, \tag{34}$$

where $\Delta\omega_S(\mathbf{k}_\parallel) = \omega(\mathbf{k}_\parallel) - \omega_S(\mathbf{k}_\parallel)$. $\Omega_S(\mathbf{k}_\parallel)$ is given by

$$(\Omega_S(\mathbf{k}_\parallel))^2 = \left(\omega_S(\mathbf{k}_\parallel) - \frac{\tilde{J}^2(\gamma^+(\mathbf{k}_\parallel))^2}{\Delta\omega_S(\mathbf{k}_\parallel)}\right)^2. \tag{35}$$

There also appears a single excitation branch in the whole 2D BZ.

IV. ANALYSIS OF THE RESULTS AND CONCLUDING REMARKS

Most of our results will be analyzed numerically due to the complexity of the equations defining the reconstruction angle and the energy of elementary excitations. Let us first examine the influence of the biquadratic interaction to the reconstruction angle by analyzing from Eq. (15) the critical value (J_S^c) of the parameter J_S for which there still exist the acceptable values of the angle θ ($0<\cos\theta<1$). One can show, using Viette formulas, that the equation has a single positive real solution for $\cos\theta$ (which can never vanish for finite values of J_S). On the other hand, the condition $\cos\theta \leqslant 1$ imposes the limitations for J_S, so that the solutions exists only for $J_S \geqslant J_S^c$, where

$$J_S^c = \frac{J}{2} + \frac{h+(2S+1)\left(D_S - \frac{\Delta K}{2}\right)}{2[1+2aS(S-1)]}. \tag{36}$$

It follows from Eq. (36) that for $S=1$, J_S^c does not depend on a, while for all other spin values ($S>1$), biquadratic interaction decreases the critical value J_S^c, i.e., favors the reconstruction. In the particular case of vanishing external field and anisotropy, J_S^c has the same value as for the bilinear interaction: $J_S^c = 0.5J$. We have presented graphical analysis for two sets of system parameters in the Figs. 3(a) and 3(b). It is important to stress that the reconstruction occurs only in the case when for $\theta \neq 0$, i.e., $J_S^c > J_S$, the energy of the reconstructed ground state $E_o(\theta)$ is lower than $E_o(0)$ for the same set of parameters. Studying the dependence $E_o = E_o(\theta)$ one can show that this function, for fixed $J_S > J_S^c$, has the maximum at $\theta=0$ and the minimum for $0<\cos\theta<1$, which is the solution of the cubic equation (15). We see that the presence of the biquadratic interaction does not disturb the stability of the reconstructed state, but that it favors it, as mentioned above. We have already mentioned in the previous section that the energy of surface excitations Ω_S in the case of reconstruction can be evaluated only numerically [Eqs. (28) and (32)]. The results of these calculations for several sets of system parameters are shown in Fig. 4,

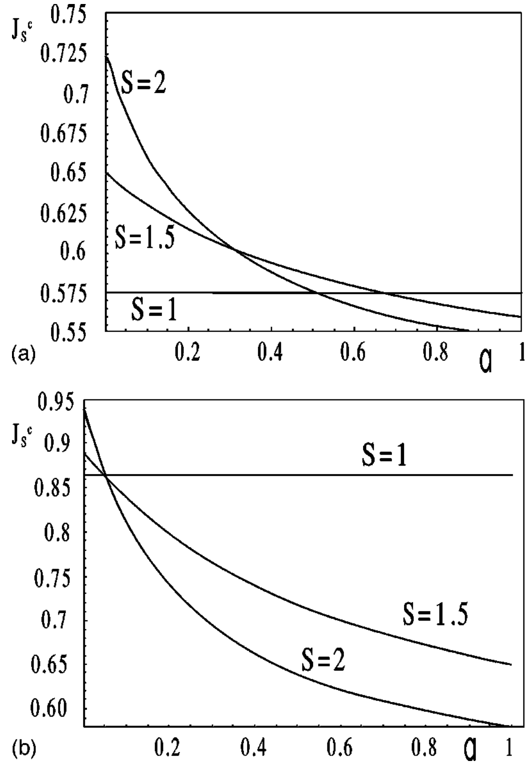

FIG. 3. The plot of the critical value of surface coupling J_S^c vs biquadratic interaction constant a for $S=1,1.5$ and 2: (a) $h=0,D_S=0.2J,\Delta K=0.1J,J=1$; (b) $h=(0.3/S)J,D_S=0.2J,\Delta K=0.1J,J=1$.

together with the bottom of the bulk continuum. Basic features of the surface excitations can be summarized in the following way:

(1) Goldstone surface mode ($\Omega_S\rightarrow 0$ for $\mathbf{k}_\parallel\rightarrow 0$) exists only in the case of vanishing external field and anisotropy [Fig. 4(a)]. It should be noted that in the long-wavelength approximation it cannot be separated from the corresponding bulk mode since both attenuation coefficients vanish $\lim_{\mathbf{k}\rightarrow 0}\eta_{1/2}\rightarrow 0$. This conclusion essentially differs from the analysis presented in Ref. 4 where Goldstone modes exist even for nonvanishing field and anisotropy.

(2) The energy of surface excitations for all analyzed sets of parameters (J_S, D_S, ΔK, and D) in the whole 2D BZ lie rather low with respect to the bottom (E_B^{bott}) of the bulk continuum, especially in the short-wave length region where the attenuation coefficients are also high so that the excitations are practically localized at the surface.

The presence of low-frequency (energy) surface waves leads to spin fluctuations with high amplitudes at and near the surface, which even at low temperatures has as a consequence the decrease of the ferromagnetic ordering of the surface which practically leads to vanishing of the antiferromagnetic ordering of the surface along the X direction. Strictly this can be shown by calculating the spin correlation functions from Green's functions for the surface. Unfortunately, the pole of the Green's function which defines the surface elementary excitation energy is the solution of at least a sixth-order equation in x $[\Delta(x)=0]$, and nothing can be achieved analytically, while numerical analysis is too com-

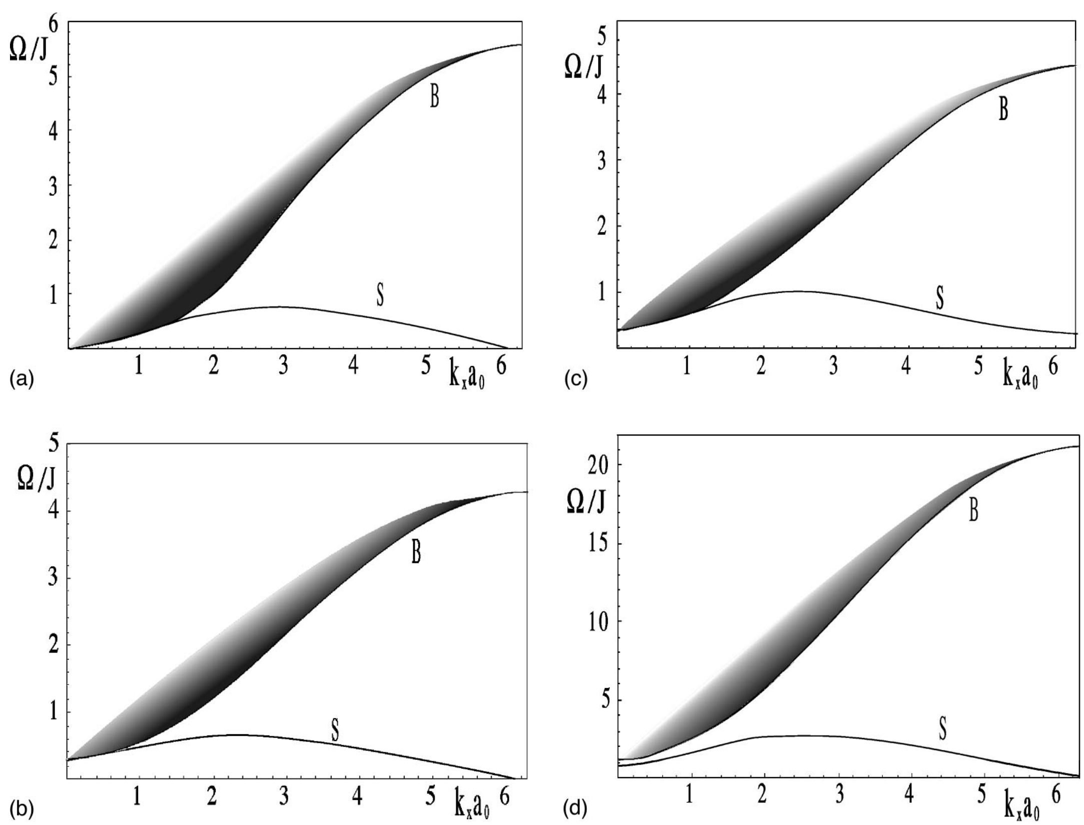

FIG. 4. The plot of the excitation energy Ω/J (surface excitations: S, bulk bottom B) along k_x direction of the Brillouin zone: (a) $S=2,h=0,J_S=0.7J,a=0.1,D=D_S=\Delta K=0,\cos\theta=0.837\,661$; (b) $S=1,h=0.3J,J_S=0.7J,a=0.1,D=D_S=\Delta K=0,\cos\theta=0.937\,67$; (c) $S=2,h=0.3J,J_S=0.6J,a=0.1,D=D_S=\Delta K=0.1J,\cos\theta=0.958\,15$; (d) $S=2,h=0.3J,J_S=0.7J,a=1,D=0.1J,D_S=0.3J,\Delta K=0.1J,\cos\theta=0.962\,836$.

plex, so we shall present the analysis of the surface magnetization in the mean-field approximation (MFA), which, although crude, confirms the above estimates.

Applying the standard MFA procedure[26] to the rotated Hamiltonian (12) (for $a=0$), from the minimum of the Gibbs' free energy we obtain the expressions for the magnetizations of the layers and additional relation for the reconstruction angle θ $(T\neq 0, \sigma_l' = \langle \hat{S}^{z'}(l)\rangle/S,\ l=0,1,2,\ldots,\ h=0)$:

$$\cos\theta(T) = \frac{J}{2J_S}\frac{\sigma_1'(T)}{\sigma_0'(T)}, \tag{37}$$

$$\sigma_l'(T) = B_S\left(\frac{\overline{\mathcal{H}_l}}{kT}\right), \tag{38}$$

where $B_S(x)$ is the Brillouin function, and for

$$l=0,\ \overline{\mathcal{H}_0} = J\sigma_1'\cos\theta - J_S\sigma_0'\cos 2\theta, \tag{39}$$

$$l=1,\ \overline{\mathcal{H}_1} = J\sigma_0'\cos\theta + J(\sigma_1'+\sigma_2'), \tag{40}$$

$$l\geqslant 2,\ \overline{\mathcal{H}_l} = J(\sigma_{l-1}'+\sigma_l'+\sigma_{l+1}'). \tag{41}$$

Additional relations for the surface layer (for unrotated components) are

$$\frac{\langle\hat{S}^z(0)\rangle}{S} \equiv \sigma_0(T) = \sigma_0'\cos\theta, \tag{42}$$

$$\langle\hat{S}^x_{a/b}(0)\rangle = \pm S\sigma_0'\tan\theta. \tag{43}$$

For $l\geqslant 1$ we have $\sigma'(l)=\sigma(l)$. Using the relation (37) the mean field at the surface $\overline{\mathcal{H}_0}$ and the first layer $\overline{\mathcal{H}_1}$ takes the form

$$\overline{\mathcal{H}_0} = J_s\sigma_0', \tag{44}$$

$$\overline{\mathcal{H}_1} = J\left[\left(1+\frac{J}{2J_S}\right)\sigma_1'+\sigma_2'\right]. \tag{45}$$

The last relations indicate that in the presence of reconstruction, the equation for the surface magnetization σ_0' becomes a self-consistent relation, decoupled from the rest of the crystal:

$$\sigma_0' = B_S\left(\frac{J_S\sigma_0'}{kT}\right), \tag{46}$$

while the relations for $\sigma_l'\equiv\sigma_l,\ l\geqslant 1$ remain coupled. The relation (46) is valid until the temperature T_C' where the reconstruction vanishes, i.e., $\theta(T_C')=0$ and which is defined by the relation

$$\sigma_0' = \sigma_0(T_C') = \frac{J}{2J_S}\sigma_1(T_C'). \tag{47}$$

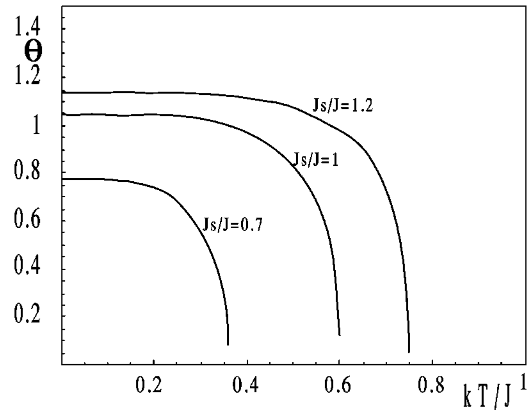

FIG. 5. Reconstruction angle θ dependence on the reduced temperature kT/J.

In the temperature region $T_C'\leqslant T\leqslant T_C$, where T_C is the bulk Curie temperature $[kT_C=(S+1)J$ for fcc$]$, the layers magnetization $\sigma_l'(T)=\sigma_l(T), l=0,1,2,\ldots$ are obtained by solving the system of coupled Eqs. (38)–(41) with $\theta=0$.

It can be easily concluded from Eq. (43) that at $T=T_C'$ the surface antiferromagnetic ordering along X direction also vanishes.

Figures 5 and 6 show the dependence of angle θ and layers magnetization $(S=1)$ on temperature, respectively. They are perfect illustrations of the behavior described above. The general conclusion is that biquadratic interaction favors the reconstruction (decreases J_S^c) but only in the case of nonvanishing external field and anisotropy. In the absence of external field and anisotropy, there occur no qualitative changes, only the normalizing factor $1+2aS(S+1)$ appears, in the expressions for energy and coefficients of sixth-order equation. Obviously, the idea of magnetic reconstruction in the surface layer only is an oversimplification, so one should introduce reconstruction in a few inner layers, probably with layer-dependent reconstruction angle. In this case one can expect a gradual transition from tilted to ferromagnetically ordered state deep in the bulk, as shown in Ref. 3, for pure Heisenberg model with antiferromagnetic next-nearest-neighbors interaction.

Our considerations of surface reconstruction can be related to the study of magnetic multilayers[27,28] where it was pointed out that biquadratic exchange and anisotropy can lead to various complicated magnetic structures. Due to current interest in magnetic multilayer systems (see, for example, the review by Allen[29]), these systems will be the subject of our further study.

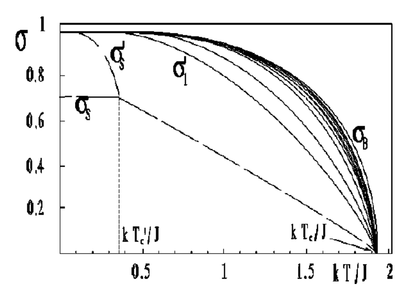

FIG. 6. Relative magnetization $\langle S^z\rangle/S$ (for $S=1$) dependence on the reduced temperature kT/J.

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APPENDIX

Equation (32) for the determination of the quantity x was obtained from the condition of vanishing of the determinant of the system (21) and (30), which has the form

$$\Delta(\kappa_1,\kappa_2)=\begin{vmatrix} \Omega-\omega_S & -\alpha_S & -\gamma^+\omega_{S1} & -\gamma^+\alpha_{S1} \\ \alpha_S & \Omega+\omega_S & \gamma^+\alpha_{S1} & \gamma^+\omega_{S1} \\ -\gamma^+\omega_{S1} & -\gamma^+\alpha_{S1} & \Delta\omega_1-\tilde{J}\gamma^+e^{-i\kappa_1} & \alpha_1 \\ \gamma^+\alpha_{S1} & \gamma^+\omega_{S1} & -\alpha_1 & -\Delta\omega_1+\tilde{J}\gamma^+e^{-i\kappa_2} \end{vmatrix}. \tag{A1}$$

Due to the economy of space, throughout the appendix, the wave-vector dependence of $\omega_S(\mathbf{k}_\parallel),\alpha_S(\mathbf{k}_\parallel),{}^+(\mathbf{k}_\parallel),\Delta\omega_1(\mathbf{k}_\parallel)$, $\omega(\mathbf{k}_\parallel)$ will be omitted. Expanding the determinant (A1) and using the expression for Ω_S (28) and auxilliary relations (31), we obtain the expression (32) for $\Delta(x)$ where the coefficients are

$$a_0=-\omega^3\Delta\omega_1,$$

$$a_1=\omega^2[\alpha_1^2-(\Delta\omega_1)^2+\gamma^{+2}(\tilde{J}^2+\alpha_{S1}^2-\omega_{S1}^2)],$$

$$a_2=\omega\{[\alpha_1^2-(\Delta\omega_1)^2+2\omega\Delta\omega_1-\tilde{J}^2\gamma^{+2}]\omega+\gamma^{+2}[\omega_S(\omega_{S1}^2+\alpha_{S1}^2)-2\alpha_S\alpha_{S1}\omega_{S1}-4\tilde{J}^2\Delta\omega_1]-\Delta\omega_1(\alpha_S^2-\omega_S^2)\},$$

$$a_3=2\gamma^{+2}(\omega_{S1}^2-\alpha_{S1}^2)(\omega^2-2\tilde{J}^2\gamma^{+2})+(4\tilde{J}^2\gamma^{+2}-\omega^2)\times[\alpha_1^2+\tilde{J}^2\gamma^{+2}-(\Delta\omega_1)^2]-\tilde{J}^2\gamma^{+2}(\omega_S^2-\alpha_S^2)+A,$$

$$a_4=(\omega_S^2-\alpha_S^2)(\tilde{J}^2\gamma^{+2}-2\omega\Delta\omega_1)+(4\tilde{J}^2\gamma^{+2}-\omega^2)\times[\alpha_1^2-(\Delta\omega_1)^2+\omega\Delta\omega_1-\tilde{J}^2\gamma^{+2}]+2\omega[2\gamma^{+2}\alpha_S\alpha_{S1}\omega_{S1}-\omega_S\gamma^{+2}(\omega_{S1}^2+\alpha_{S1}^2)]+A,$$

$$a_5=(4\tilde{J}^2\gamma^{+2}-\omega^2)\gamma^{+2}(\omega_{S1}^2-\alpha_{S1}^2)+\tilde{J}^2\gamma^{+2}(\omega_S^2-\alpha_S^2)-A,$$

$$a_6=(\alpha_S^2-\omega_S^2)(\tilde{J}^2\gamma^{+2}-\omega\Delta\omega_1)+\omega[\gamma^{+2}\omega_S(\omega_{S1}^2+\alpha_{S1}^2)-2\gamma^{+2}\alpha_S\alpha_{S1}\omega_{S1}]-A,$$

$$A=(\omega_S^2-\alpha_S^2)[(\Delta\omega_1)^2-\alpha_1^2]+\gamma^{+4}(\omega_{S1}^2-\alpha_{S1}^2)^2+2\gamma^{+2}(\omega_{S1}^2+\alpha_{S1}^2)(\omega_S\Delta\omega_1+\alpha_1\alpha_S)-4\gamma^{+2}\alpha_{S1}\omega_{S1}(\omega_S\alpha_1+\alpha_S\Delta\omega_1).$$

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